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Monte Carlo simulation of hot-carrier phenomena in open quantum devices: A kinetic approach / PROIETTI ZACCARIA, Remo; Iotti, Rita Claudia; Rossi, Fausto. - In: APPLIED PHYSICS LETTERS. - ISSN 0003-6951. - STAMPA. - 84:1(2004), pp. 139-141. [10.1063/1.1637965]

Availability:

This version is available at: 11583/1405263 since:

Publisher:

AIP American Institute of Physics

Published

DOI:10.1063/1.1637965

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Citation: *Appl. Phys. Lett.* **84**, 139 (2004); doi: 10.1063/1.1637965

View online: <http://dx.doi.org/10.1063/1.1637965>

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Monte Carlo simulation of hot-carrier phenomena in open quantum devices: A kinetic approach

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(Received 28 July 2003; accepted 9 November 2003)

An alternative simulation strategy for the study of nonequilibrium carrier dynamics in quantum devices with open boundaries is presented. In particular, we propose replacing the usual modeling of open quantum systems based on phenomenological injection/loss rates with a kinetic description of the system-reservoir thermalization process. More specifically, in this simulation scheme the partial carrier thermalization induced by the device spatial boundaries is treated within the standard Monte Carlo approach via an effective scattering mechanism between the highly nonthermal device electrons and the thermal carrier distribution of the reservoir. The proposed simulation strategy is applied to state-of-the-art semiconductor nanostructures. © 2004 American Institute of Physics. [DOI: 10.1063/1.1637965]

Continuous progress in microelectronics technology pushes device miniaturization toward limits where the traditional semiclassical transport theory¹ can no longer be applied, and more rigorous quantum-transport approaches are required.² However, in spite of the quantum-mechanical nature of carrier dynamics in the core region of typical nanostructured devices—like semiconductor superlattices and double-barrier structures—the overall behavior of such quantum systems is often the result of a nontrivial interplay between phase coherence and energy relaxation/dephasing,³ the latter being primarily due to the presence of spatial boundaries. It follows that a proper treatment of these nanoscale devices requires a theoretical modeling able to properly account for both coherent and incoherent—i.e., phase-breaking—processes on the same footing. In this spirit, a generalization to open systems—i.e., systems with open boundaries—of the well known Semiconductor Bloch Equations (SBE)⁴ has been recently proposed.⁵ However, such fully microscopic treatments—which are essential for the basic understanding of the quantum phenomena involved—are extremely computer-time consuming, and therefore cannot be employed in standard optoelectronic-device modeling/optimization. In contrast, to this end partially phenomenological models are usually considered. Among such simulation strategies it is worth mentioning the approach recently proposed by Fischetti and co-workers.⁶ Within such partially phenomenological treatments the coupling of the quantum device with external reservoirs is usually described in terms of extremely simplified injection/loss models.⁶

Our aim in this letter is to present an innovative simulation strategy for the study of nonequilibrium carrier dynamics in quantum devices with open boundaries: what we propose is to replace the usual modeling of open quantum systems based on phenomenological injection/loss rates with a kinetic description of the system-reservoir thermalization process; in particular, within this simulation scheme the partial carrier thermalization induced by the device spatial boundaries will be treated via a conventional Monte Carlo (MC) approach in terms of an effective scattering mechanism

between the highly nonthermal device electrons and the thermal carrier distribution of the reservoir. As we shall see, in our approach the total number of simulated electrons is preserved (closed scheme); this is a distinguished advantage of the proposed strategy, compared to hybrid—direct numerical-integration plus MC-sampling—schemes, where the total number of particles is not constant (open scheme).

As a starting point, let us recall the usual approach used for the simulation of state-of-the-art semiconductor-based quantum devices. By denoting with f_α the carrier distribution over the electronic states α of the device, the equation governing hot-carrier transport/relaxation phenomena in open systems can be schematically written as

$$\frac{d}{dt}f_\alpha = \left. \frac{d}{dt}f_\alpha \right|_{\text{scat}} + \left. \frac{d}{dt}f_\alpha \right|_{\text{res}}. \quad (1)$$

The first term describes scattering dynamics within the device active region and is usually treated at a kinetic level via a Boltzmann-like collision operator of the form

$$\left. \frac{d}{dt}f_\alpha \right|_{\text{scat}} = \sum_{\alpha'} (P_{\alpha\alpha'}^s f_{\alpha'} - P_{\alpha'\alpha}^s f_\alpha), \quad (2)$$

where $P_{\alpha\alpha'}^s$ denotes the total (summed over all relevant interaction mechanisms) scattering rate from state α' to state α .

The last term in (1) accounts for the open character of the system, i.e., it describes injection/loss contributions from/to external carrier reservoirs. This is usually treated via a relaxation-time-like term of the form⁶

$$\left. \frac{d}{dt}f_\alpha \right|_{\text{res}} = -\gamma_\alpha(f_\alpha - f_\alpha^\circ) = G_\alpha - \gamma_\alpha f_\alpha, \quad (3)$$

where γ_α^{-1} can be regarded as the device transit time for an electron in state α and f_α° is the carrier distribution in the external reservoirs; the latter may correspond to two distinct quasi-equilibrium distributions (left and right chemical potentials), or may describe a generic nonequilibrium distribution within the external reservoirs. As anticipated, in spite of

the kinetic nature of the scattering dynamics in (2), the last (relaxation-time-like) term in (3) describes carrier injection/loss on a partially phenomenological level; this, in turn, requires hybrid simulation strategies⁷ combining a MC sampling of the scattering dynamics with a direct numerical integration of injection/loss terms.

In this Letter we propose to replace the conventional relaxation-time term in (3) with a Boltzmann-like operator of the form

$$\left. \frac{d}{dt} f_\alpha \right|_{\text{res}} = \sum_{\alpha'} (P_{\alpha\alpha'}^r f_{\alpha'} - P_{\alpha'\alpha}^r f_\alpha). \quad (4)$$

The latter has exactly the structure of the scattering operator in (2); however, the new scattering rates $P_{\alpha\alpha'}^r$ describe electronic transitions within the simulated region induced by coupling with external carrier reservoirs. We stress that, contrary to the conventional injection/loss term in (3), in this case there is no particle exchange between the device active region and thermal reservoirs; it follows that the total number of simulated particles is preserved.

Let us now discuss the explicit form of the scattering rates $P_{\alpha\alpha'}^r$ in Eq. (4). In the absence of scattering processes ($P_{\alpha\alpha'}^s = 0$), the steady-state solution of the conventional injection/loss model in (3) is $f_\alpha = f_\alpha^\circ$. As a first requirement, we impose the same steady-state solution ($f_\alpha = f_\alpha^\circ$) to the new collision operator in (4), which in turn will impose conditions on the explicit form of the scattering rates $P_{\alpha\alpha'}^r$. More specifically, from the detailed-balance principle¹ we get

$$\frac{P_{\alpha\alpha'}^r}{P_{\alpha'\alpha}^r} = \frac{f_\alpha^\circ}{f_{\alpha'}^\circ}. \quad (5)$$

It follows that our transition rates should be of the form

$$P_{\alpha\alpha'}^r = \mathcal{P}_{\alpha\alpha'} f_{\alpha'}^\circ, \quad (6)$$

where \mathcal{P} can be any positive and symmetric transition matrix ($\mathcal{P}_{\alpha\alpha'} = \mathcal{P}_{\alpha'\alpha} > 0$). Indeed, it is well known that in steady-state conditions what is important is the ratio of the scattering rates in (5) and not their absolute values. The latter, in contrast, are crucial in determining the transient nonequilibrium response of the system. Since our aim is to replace the injection/loss term in (3) with the Boltzmann-like term in (4), as a second requirement we shall then ask that the typical relaxation dynamics induced by the new collision term corresponds to the phenomenological relaxation times in (3). More precisely, we shall impose that the total out-scattering rate—summed over all possible final states—coincides with the relaxation rates γ_α :

$$\Gamma_\alpha \equiv \sum_{\alpha'} P_{\alpha'\alpha}^r = \gamma_\alpha. \quad (7)$$

By assuming—as the simplest form of the symmetric transition matrix in (6)— $\mathcal{P}_{\alpha\alpha'} = p_\alpha p_{\alpha'}$, Eq. (7) reduces to the following system of equations for p_α :

$$\sum_{\alpha'} p_{\alpha'} f_{\alpha'}^\circ = \frac{\gamma_\alpha}{p_\alpha}. \quad (8)$$

Since the sum on the left is α -independent, we immediately get $p_\alpha \propto \gamma_\alpha$. Starting from this result, we finally obtain

$$\mathcal{P}_{\alpha\alpha'} = p_\alpha p_{\alpha'} = \frac{\gamma_\alpha \gamma_{\alpha'}}{\sum_{\alpha''} \gamma_{\alpha''} f_{\alpha''}^\circ}. \quad (9)$$

Equation (6) together with Eq. (9) provides the explicit form of the desired system-reservoir scattering rates entering the Boltzmann-like collision term in (4). As anticipated, the proposed kinetic formulation, which involves Boltzmann-like collision operators only, is particularly suited for a standard Ensemble-MC simulation approach, where one deals with a fixed number of particles. In this respect, it is worth noticing that, contrary to the phenomenological model in Eq. (3), in the proposed closed-system formulation the total carrier density is not fixed by the external reservoirs (the resulting transport equation is homogeneous).

In order to test the viability of the proposed simulation strategy, we have developed a fully three-dimensional (3D) MC simulator, using as basis states α the product of scattering states along the field/growth direction and two-dimensional plane waves. In addition to the new scattering-like thermalization mechanism in (4), to properly describe phonon-induced energy/momentum relaxation within the device active region, carrier-phonon scattering has been treated in a fully 3D fashion.

As a starting point, we have considered an extremely simple transport problem: a GaAs mesoscopic bulk system of length $l = 200$ nm sandwiched between two reservoirs with different chemical potentials ($\mu_{\text{left}} - \mu_{\text{right}} = 50$ meV). We have applied to this problem the simulation strategy previously described [see Eq. (4)], comparing the results with those of the conventional simulation approach [see Eq. (3)].

Figure 1(a) shows the transient carrier dynamics—from 1 ps (dashed curve) to 9 ps (a thick solid curve) at steps of 1 ps (thin solid curves)—resulting from the conventional injection/loss model in (3). Here, we show the time evolution of the carrier distribution in momentum space. Since within this model we start from an empty-device configuration, the simulated experiment shows a progressive increase of the carrier distribution, which from the very beginning exhibits a strong left–right asymmetry due to the chemical-potential misalignment. This scenario clearly shows the open nature of the conventional approach, which does not allow the direct use of a standard MC procedure.

Figure 1(b) shows again the transient evolution of the carrier distribution in momentum space, but obtained from the proposed simulation approach. As anticipated, in this case we deal with a fixed number of particles which at time $t = 0$ are arbitrarily chosen to be equally distributed in the 3D momentum space. Moreover, the total carrier density, which is now a free parameter, has been set equal to the steady-state value in (a) (which can be directly evaluated from the thermal distribution f_α°). Contrary to the time evolution in (a), here at very short times the device region is already occupied and its charge distribution in momentum space is more symmetric. Only at later times, due to the effective scattering mechanism in (6), we recover the asymmetric distribution of Fig. 1(a) (see the solid curve).

Figure 1(c) shows the charge current density as a function of time corresponding to the two simulated experiments

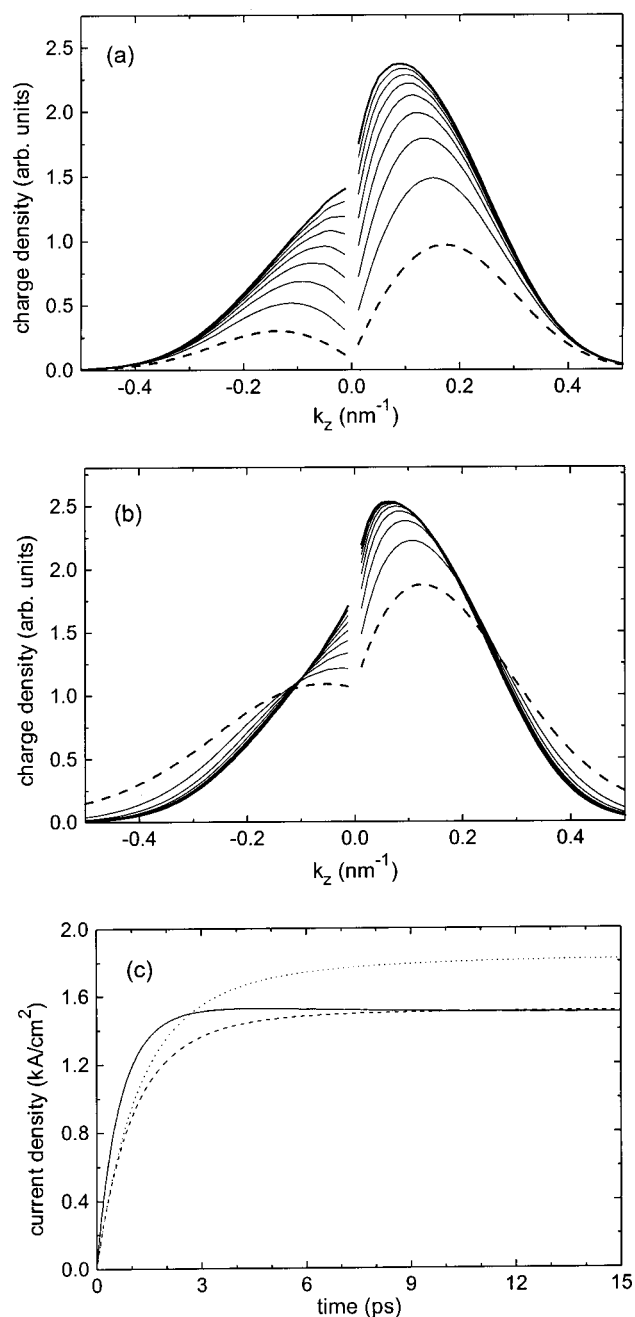


FIG. 1. Room-temperature transport properties of a GaAs mesoscopic bulk system of length $l = 200$ nm sandwiched between two reservoirs with different chemical potentials ($\mu_{\text{left}} - \mu_{\text{right}} = 50$ meV). Transient dynamics of the carrier distribution in momentum space—from 1 ps (dashed curve) to 9 ps (solid curve)—as obtained (a) from the conventional injection/loss model in (3) and (b) from the proposed simulation strategy. (c) Charge current density as a function of time corresponding to the two simulated experiments in (a) (dashed curve) and (b) (solid curve). The scattering-free or ballistic result (dotted curve) is also reported.

in (a) (dashed curve) and (b) (solid curve). At time $t = 0$ the current is in both cases equal to zero; this is however ascribed to different reasons: in (a) at $t = 0$ the carrier density is equal to zero while the drift velocity is different from zero; in (b) the drift velocity is equal to zero while the carrier density is different from zero. In spite of a slightly different transient, both curves reach almost the same steady-state value, confirming the validity of the proposed simulation strategy. We finally stress that the steady-state condition pre-

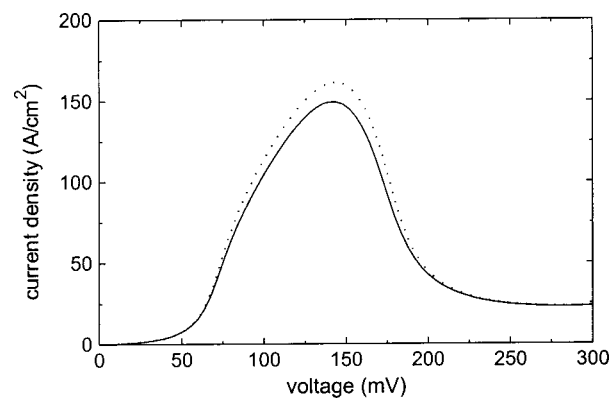


FIG. 2. Room-temperature current-voltage characteristics of a GaAs/AlGaAs resonant-tunnelling diode (with barrier height 0.24 eV and barrier width and separation of 2.8 and 4.4 nm, respectively) as obtained from our MC simulation scheme with (solid curve) and without (dotted curve) carrier-phonon scattering.

viously mentioned is the result of a strong interplay between thermalization induced by the external reservoirs and phonon-induced momentum relaxation within the device active region. Indeed, in the phonon-free case (dotted curve) the steady-state current—which is fully ballistic—reaches significantly higher values. The momentum-relaxation dynamics previously mentioned is clearly visible in Fig. 1(a), where the peaks of the injected carrier distribution (see dashed curve) are progressively shifted to lower wavevectors (see solid curve).

As a second testbed, we have considered a prototypical semiconductor quantum device: a GaAs/AlGaAs resonant-tunnelling diode with a barrier height of 0.24 eV and a barrier width and separation of 2.8 and 4.4 nm. Figure 2 shows the current-voltage characteristics obtained from the proposed MC simulation scheme with (solid curve) and without (dotted curve) carrier-phonon scattering. As we can see, we are able to properly describe the typical resonance scenario. More specifically, as expected, in the presence of phase-breaking processes—like carrier-phonon scattering—the resonance peak is significantly reduced. Also in this case the proposed simulation strategy comes out to properly describe the key phenomena under investigation.

In summary, we have proposed an alternative simulation strategy for the study of hot-carrier phenomena in open quantum devices. By replacing the conventional injection/loss model with a Boltzmann-like effective scattering operator, we are able to move from an open to a closed scheme, a prerequisite for the application of the well-established Ensemble MC method. The simulated experiments based on this approach have fully confirmed its validity as well as its power and flexibility.

¹See, e.g., C. Jacoboni and P. Lugli, *The Monte Carlo Method for Semiconductor Device Simulations* (Springer-Verlag, Wien, 1989).

²See, e.g., *Theory of Transport Properties of Semiconductor Nanostructures*, edited by E. Schöll (Chapman & Hall, London, 1998).

³See, e.g., R. C. Iotti and F. Rossi, *Phys. Rev. Lett.* **87**, 146603 (2001).

⁴See, e.g., F. Rossi and T. Kuhn, *Rev. Mod. Phys.* **74**, 895 (2002), and references therein.

⁵R. Proietti Zaccaria and F. Rossi, *Phys. Rev. B* **67**, 113311 (2003).

⁶M. V. Fischetti, *Phys. Rev. B* **59**, 4901 (1999), and references therein.

⁷See, e.g., R. C. Iotti and F. Rossi, *Appl. Phys. Lett.* **76**, 2265 (2000).